GAPS IN TOXIC INDUSTRIAL CHEMICAL (TIC) MODEL SYSTEMS

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Reasons for Concerns

- Recent increased threat of terrorist attacks on industrial facilities and modes of transportation
- Occurrence of a few major railcar accidents with casualties in the past few years. Many more casualties are predicted by the model system than are observed.
- Some aspects of the modeling system are not well known. This paper addresses those “gaps”

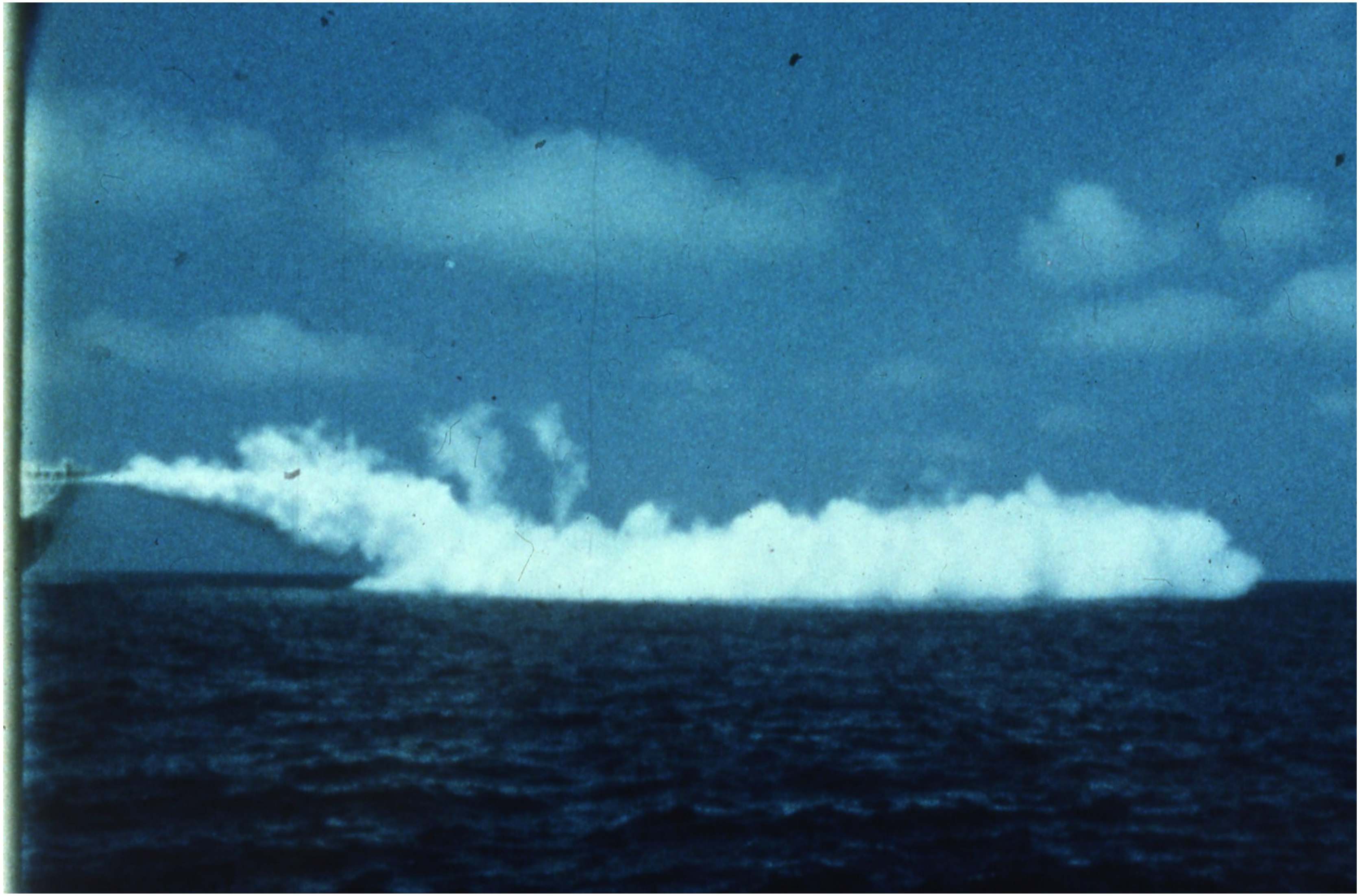
Major Interest in Chlorine, Anhydrous Ammonia, and Sulfur Dioxide

- Stored and transported as pressurized liquefied gas in large quantities
- Have low boiling point and thus rapidly volatilize when released from storage tank to the atmosphere
- Cause inhalation health effects at relatively low concentrations

Comprehensive Model System (from Scenario Definition Module to Health Effects Module)

- Scenario definition
- Source emissions model
- Transport and dispersion model (including initial jet algorithm, source blanket or mist pool, dense gas slumping, building effects, and turbulent dispersion)
- Removal processes (gravitational settling of drops, dry deposition, chemical reactions)
- Population exposure model (concentration or dosage integrated over the population) and health risk model

Release of LNG from back of tanker onto water



Desert Tortoise 2 Anhydrous Ammonia Release
(Controlled Field Experiment)

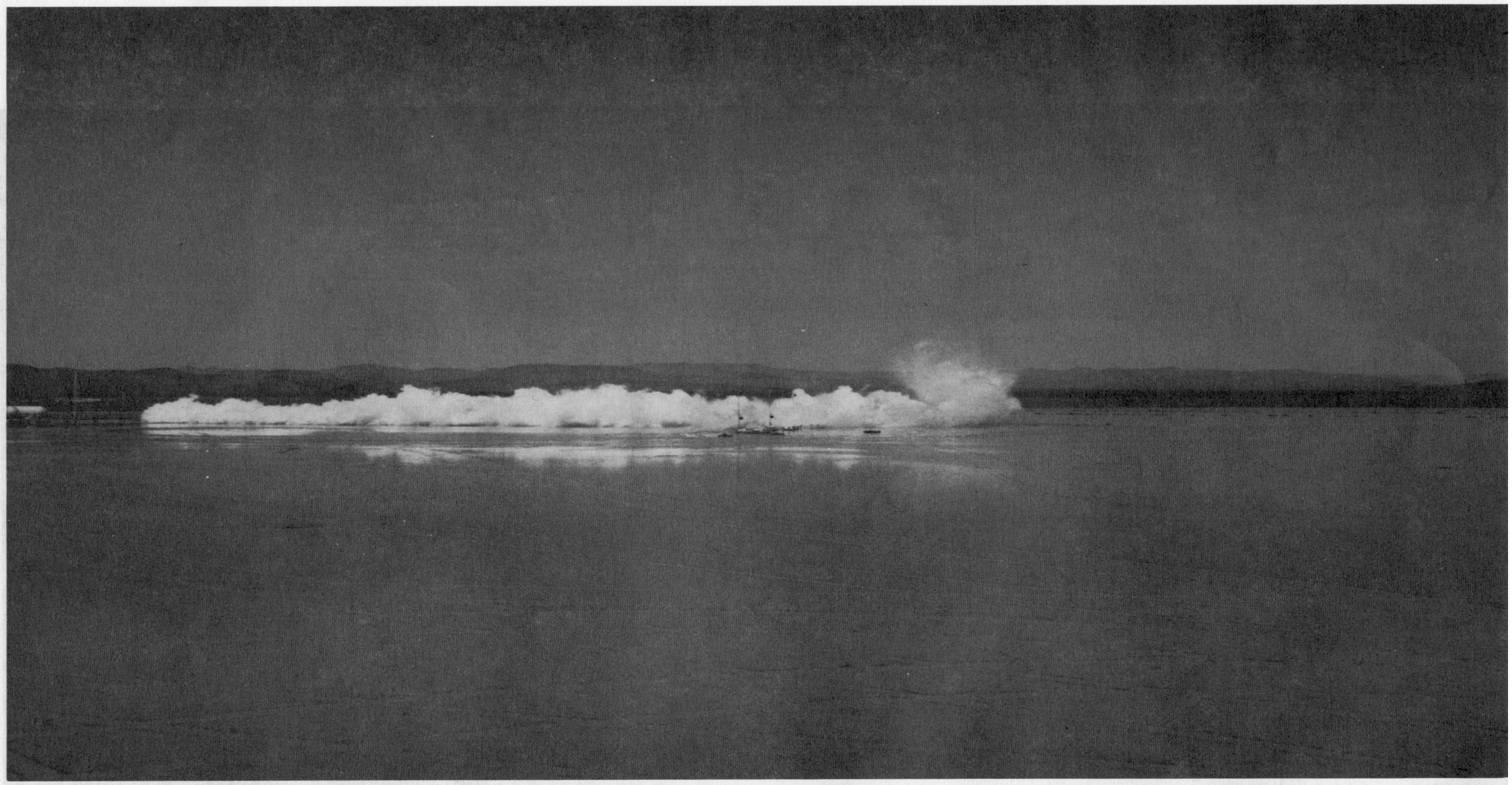


Fig. 17. Desert Tortoise 2 (crosswind wide angle camera). Time = 35 s.

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Why are there not more casualties?

- Model-predicted concentrations would suggest more casualties than are observed
- The very large and dense release may form a persistent cloud over the source that may follow terrain drainage and may only slowly be transported away.
- In urban and industrial areas, the dense cloud may be affected by the obstacles.
- The models tend to ignore removal by chemical reactions and deposition, which can be very significant.
- The TIC health limits may be conservative.

Gap 1 - Release scenario definition

- Easier for industrial facility (known location and physical conditions) than for transportation accident (random location and poorly known physical conditions)
- Hole (or holes) sizes, shapes, and locations are not well known, even months after an incident
- Local small-scale topo, buildings and other obstacles, and underlying surface info are difficult to find and sometimes are not available at all
- Local (on-site) meteorology is seldom available

Gap 2 – Source Terms

- Magnitude and duration of release, and chemical and physical properties
- Release rate is largest for liquid phase, smallest for gas phase, and intermediate for two phase
- Most scenarios of interest are two phase (e.g., chlorine, stored as a pressurized liquefied gas), which has been studied by researchers for decades with uncertainties remaining.
- Much depends on vessel level swell (foaming)
- Droplet sizes (in two-phase releases) determine how much will “rain-out” or will move downwind.
- The jet must be modeled as its pressure reduces to ambient and is handed off to the dispersion model.

Gap 3 – Transport and Dispersion

- T&D calculations depend on specification of averaging time for effects (health, materials, vegetation), e.g., 20 sec for chlorine
- T&D models run the range from simple slab models (e.g., HGSYSTEM) to CFD models (e.g., FLACS)
- Different T&D models “begin” and “end” at different places in the model system (e.g., some directly link with source models)

Gap 3 – T&D Models Point 1 – Initial cloud spread when very dense and low winds

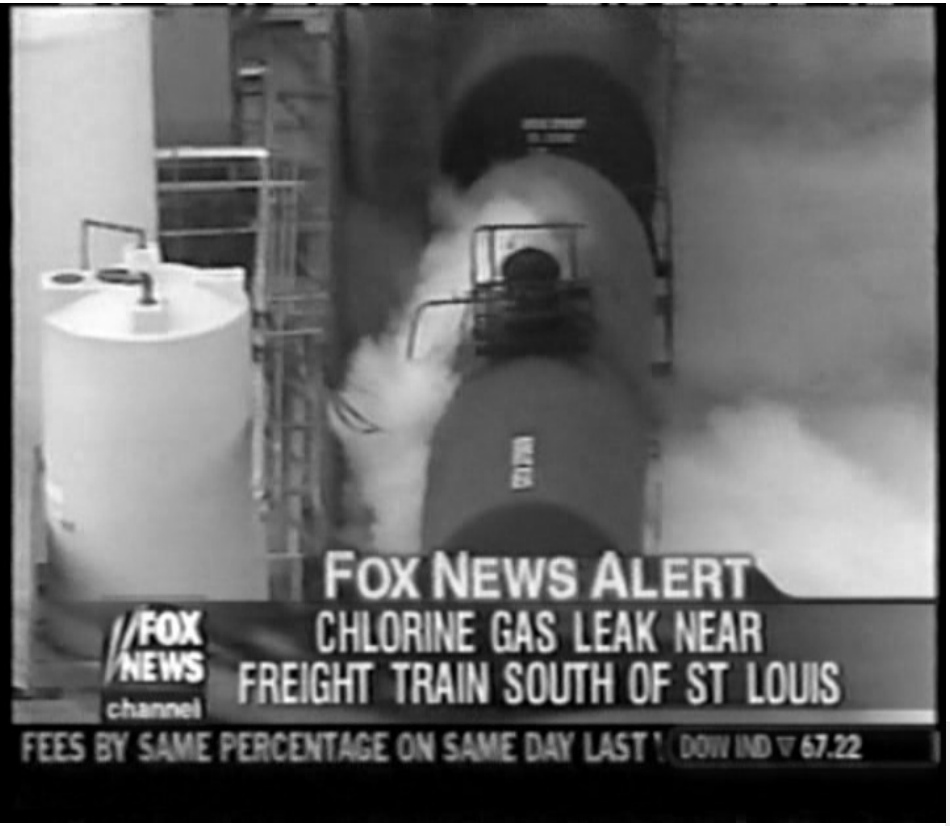
- Current models (e.g., SLAB, PHAST) account for reduced entrainment and transport velocity for large dense clouds
- But for very large and dense clouds, such as the 80 tons of two-phase chlorine emitted from a large hole in a railcar, and for light winds, the cloud may stay near the source as a persistent mist pool and only slowly be entrained in the ambient air flow.
- There are no field experiments involving this situation and plans are underway for such experiments

Gap 3 – T&D Models Point 2 – Terrain and Obstacle Effects

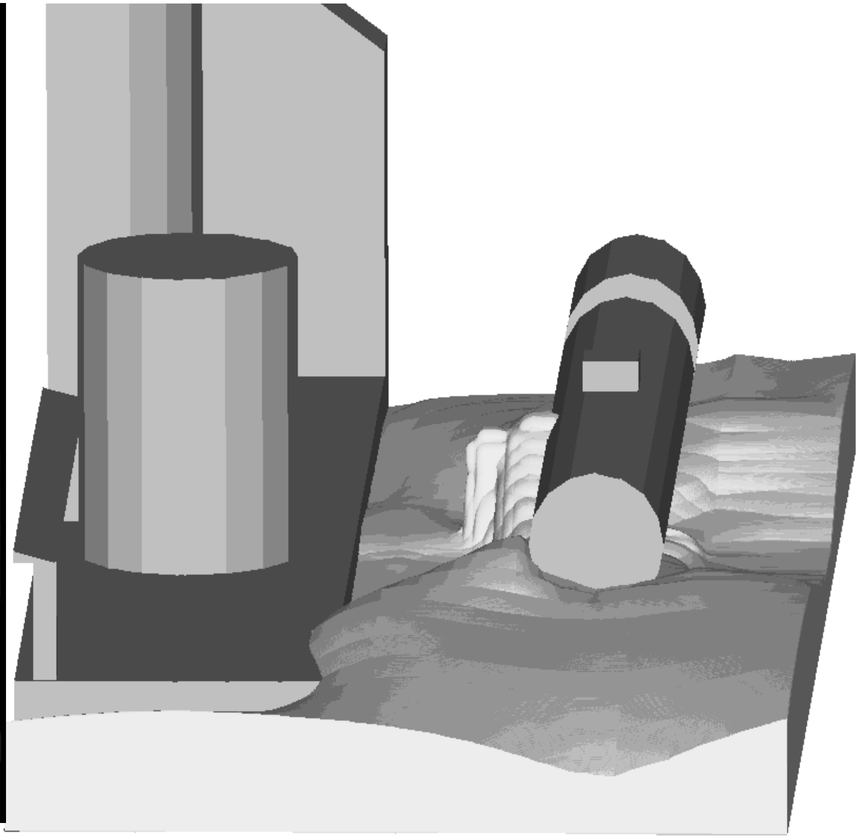
- Most models assume flat terrain or simple slopes
- Actual release scenarios inevitably involve ditches and hills and obstacles (tanks, buildings, trees)
- Some CFD (FLACS, Fluent, FEM3) and diagnostic wind models (QUIC) can treat 3-D building and terrain, if inputs are available
- See FLACS application to Festus and Chicago scenario (e.g., showing jet hitting railcar, and hold-up in building wakes)

Examples of terrain and obstacle effects for Festus and Chicago chlorine scenarios

- Festus – We estimated local geometry (including buildings, tanks, and trees) from videos of the accident
- Chicago hypothetical release
  - Flat terrain except for Chicago river and Lake Michigan being 2 m below land level.
  - 3D high-resolution building files



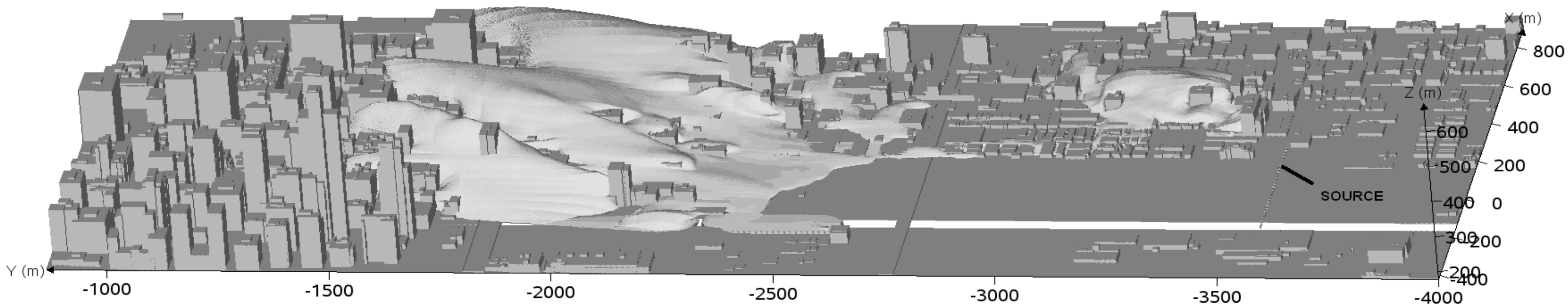
Observed



FLACS CFD Model

Chlorine cloud at Festus, Missouri

Railroad junction in Chicago, looking towards the east-northeast. The release is near the middle. T



FLACS CFD model simulation of 100 ppm contour for Chicago hypothetical release scenario

Gap 4 – Removal processes

- Chemical reactions are significant for the top-three TICs - chlorine, ammonia, and sulfur dioxide
- Photolysis (due to solar energy) can remove much chlorine gas
- Gravitational settling of larger drops
- Dry deposition of gas and small drops (v_d = 1 to 5 cm/s for chlorine, which can remove much chlorine (50 % of chlorine mass in first 100 m for stable light wind ambient conditions)
- Sensitivity studies with current models confirm large removal
- Small-scale experiments are planned (such as filling a chamber with chlorine gas and estimating its rate of deposition on certain types of soils or vegetation)

Deposition sensitivity studies

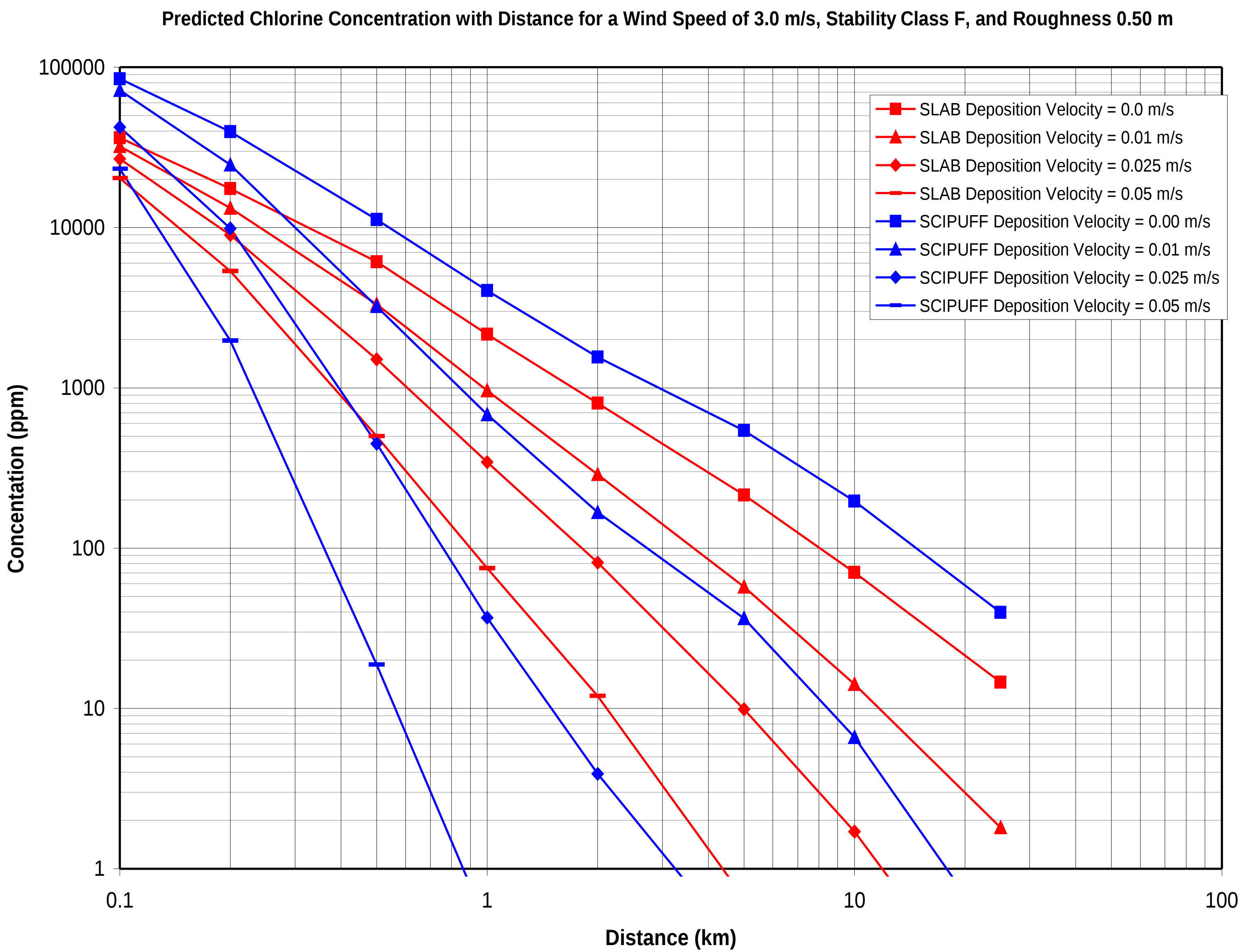
- Because of questions regarding possible removal of cloud mass by dry deposition and/or chemical reactions, an analytical analysis was done and the SCIPUFF and SLAB models were run for the Chicago scenario with four assumed dry deposition velocities (0.0, 1, 2.5, and 5 cm/s)
- Sensitivity runs were also made with surface roughnesses of 3, 10, and 50 cm, wind speeds of 0.25, 0.5, 1, 2, and 3 m/s, and stability classes D, E and F

Analytical solution for removal by dry deposition at the ground surface for ground level sources
Note that the deposition velocity v_d for chlorine is relatively large (1 to 5 cm/s)

$$Q(x)/Q(0) = [\exp(\int(dx/\sigma_z)]-(\sqrt{(2/\pi)})v_d/u$$

For u = 1 m/s and a deposition velocity, v_d, of 1 cm/s (i.e., v_d/u = 0.01), the distances, x (50%), are

Stability	A and B	C	D	E	F
σ_z @ x=1km	**> 100 m**	**55 m**	**30 m**	**18 m**	**12 m**
x 50%	**> 10 km**	**1.8 km**	**0.4 km**	**0.15 km**	**0.10 km**



Modeled chlorine concentrations downwind of the hypothetical railcar release for the "base case", illustrating the effect of including deposition in SCIPUFF and SLAB simulations.

Gap 5 – Exposure and Health Risk

- Population distribution as function of time of day
- Fraction of population indoors and use of models for indoor concentrations as a function of outdoor concentration and air exchange rate
- Toxic load relations (for chlorine, for the same dosage, the health effects are worse if the dosage takes place at high concentrations over a short time rather than low concentrations over a long time)
- Health effects studies are based mostly on animal data and not on human data
- A degree of conservatism (a safety factor) may be built into the health risk relations

Planned field and laboratory experiments

- To address the gaps, a series of field and laboratory experiments is being planned
- Issues with safety cause us to consider surrogate chemicals with behavior similar to chlorine
- When can small-scale experiments be satisfactorily scaled up?
- Teams of experts in each area are assisting with the planning